Reactive Carbon Capture:
Status, Challenges, and Opportunities

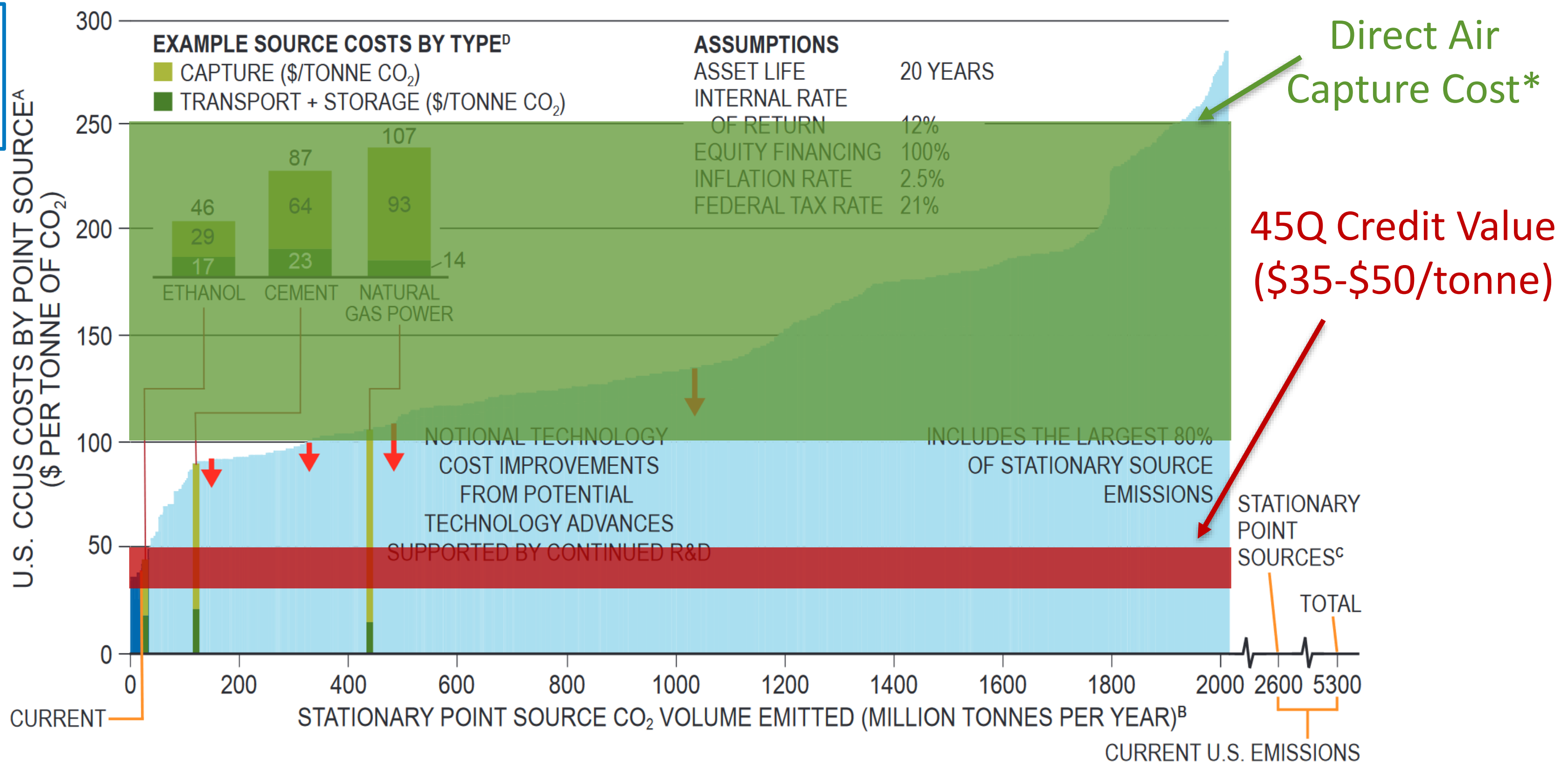
Josh Schaidle

February 3rd, 2022

ARPA-E Reactive Carbon Capture Workshop

Cost Curve for CO_2 Capture and Storage in the US

$100/t CO_2 = $1/gallon of gasoline



National Petroleum Council, *Meeting the Dual Challenge, A Roadmap to At-Scale Deployment of Carbon Capture, Use, and Storage*, 2019

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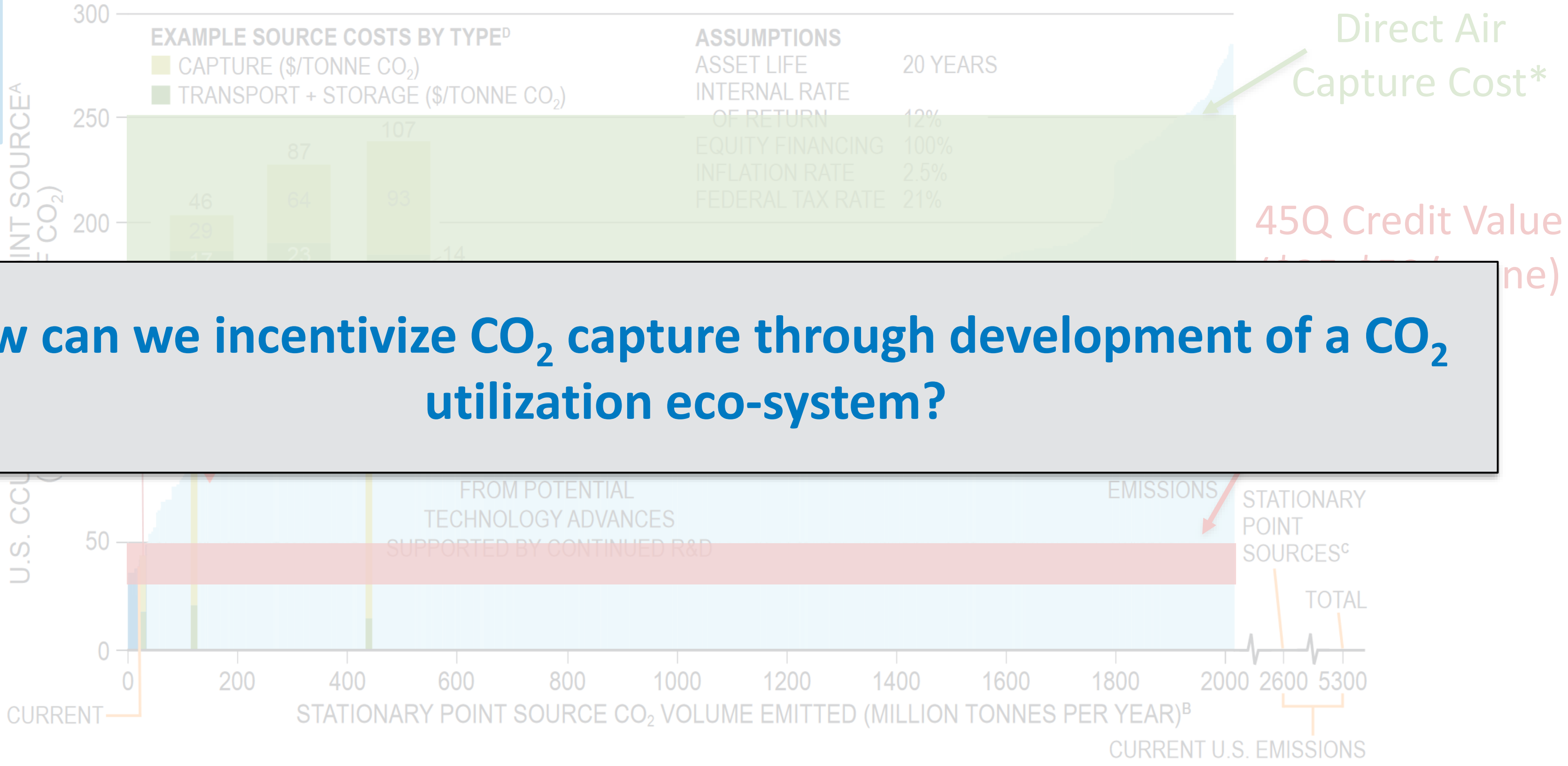

How can we incentivize CO_2 capture through development of a CO_2 utilization eco-system?

National Petroleum Council, *Meeting the Dual Challenge, A Roadmap to At-Scale Deployment of Carbon Capture, Use, and Storage*, 2019

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Emerging Approach: Reactive Capture of CO_2

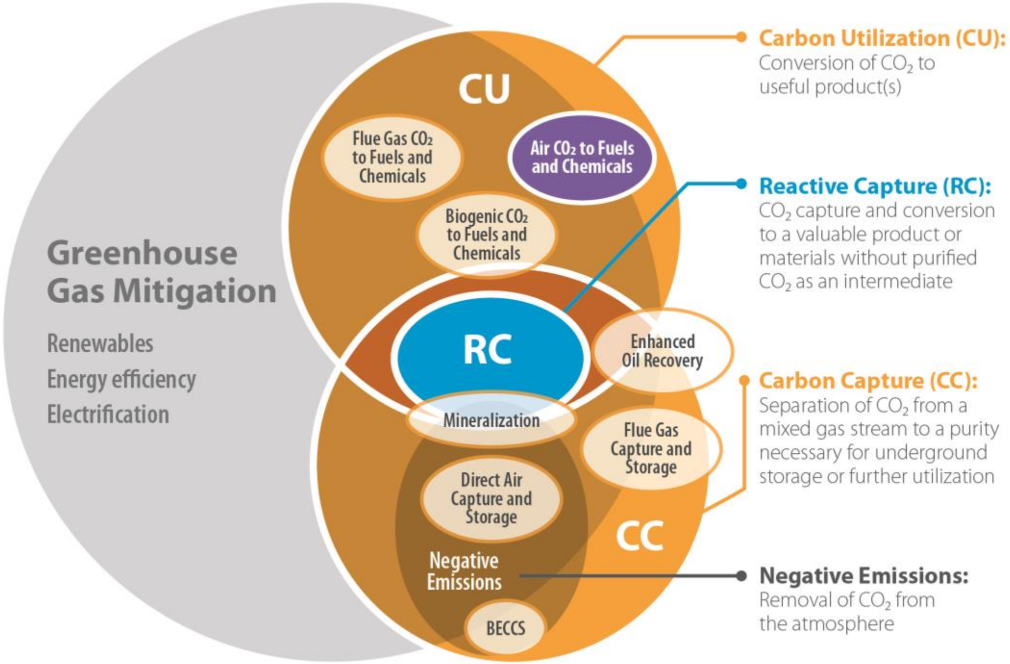
Reactive Capture Definition: The coupled process of capturing CO_2 from a mixed gas stream and converting it into a valuable product *without* going through a purified CO_2 intermediate

Can Include:

- Integration of CO_2 separation and conversion in one step
- Integration of separation and conversion in one unit
- Process intensification

Product Targets:

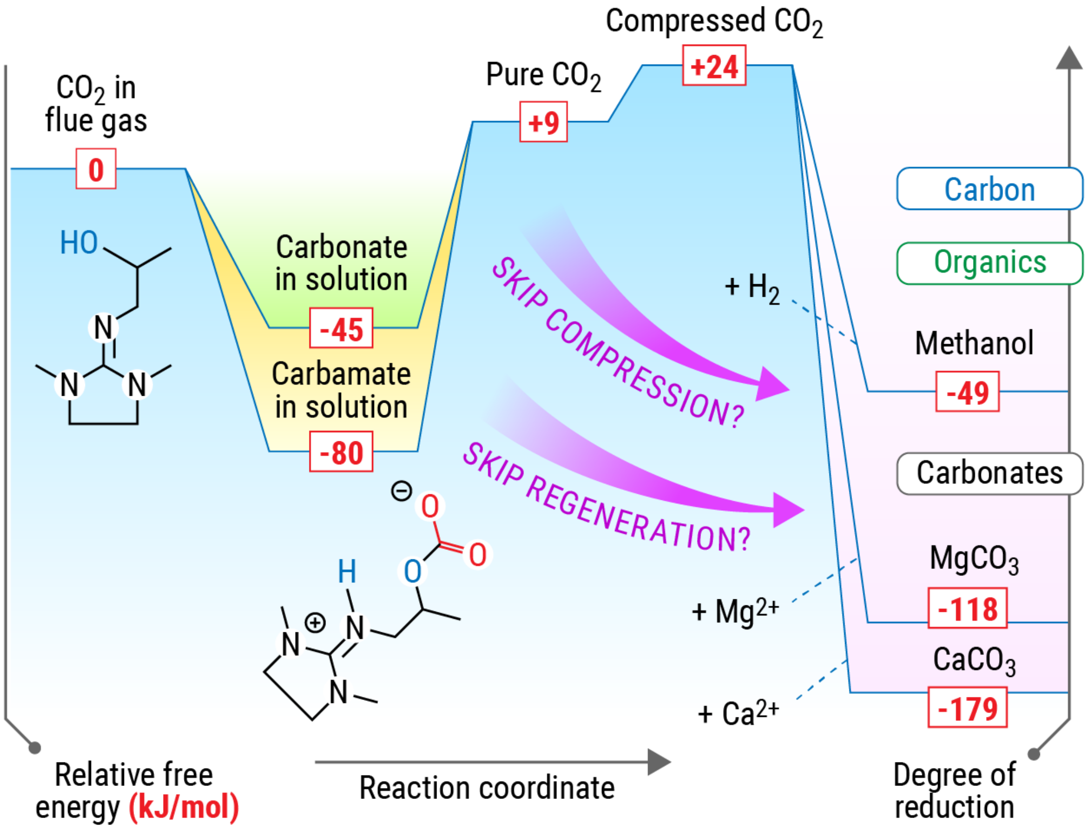
Must form a valuable product, or mixture of products, in a more reduced state than CO_2



Summary Report of the Reactive CO2 Capture: Process Integration for the New Carbon Economy Workshop, February 18-19, 2020 (https://www.nrel.gov/docs/fy21osti/78466.pdf)

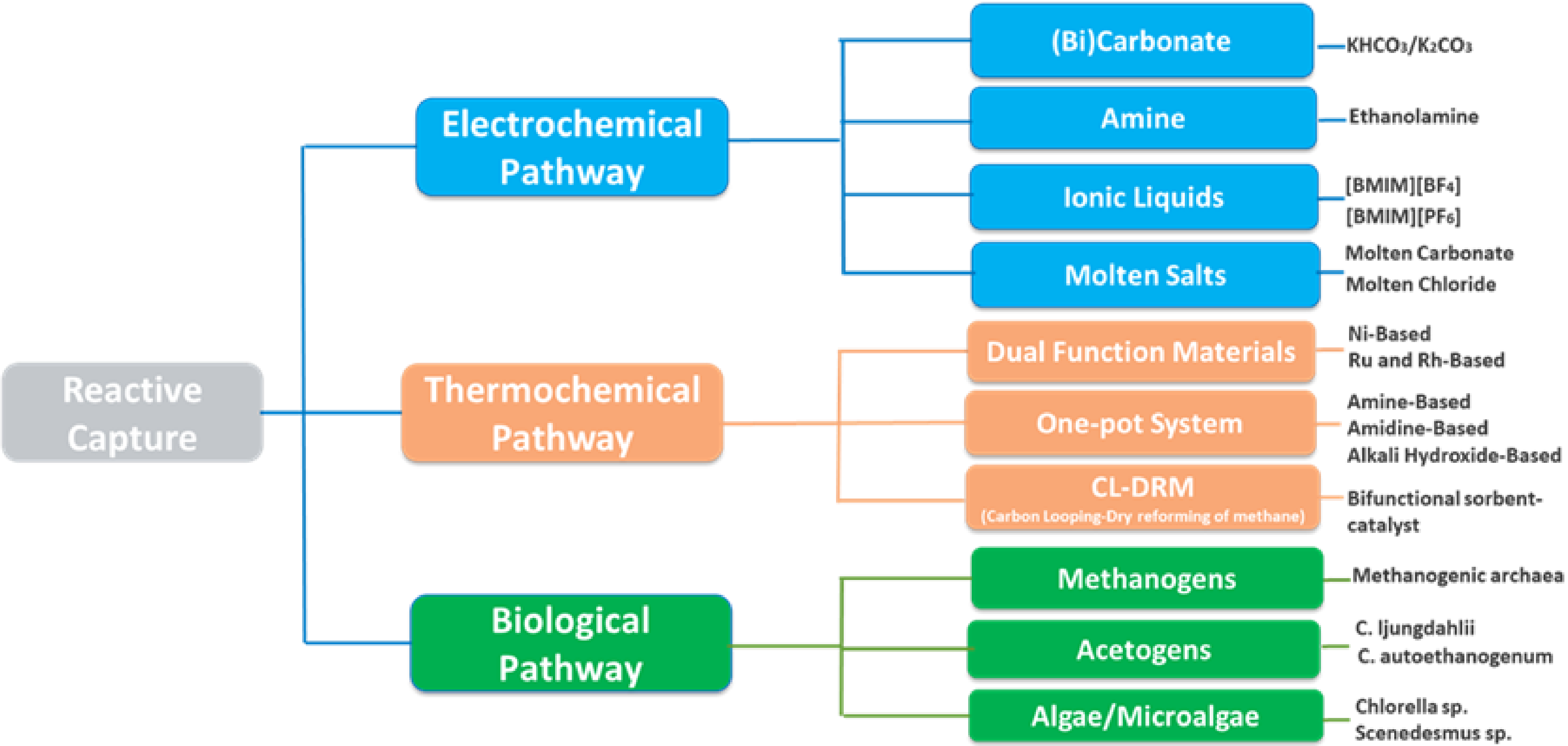
Why Reactive Capture?

Avoid the energy input required to capture, purify, and compress CO_2



Courtesy of David Heldebrant and Joshuah Stolaroff

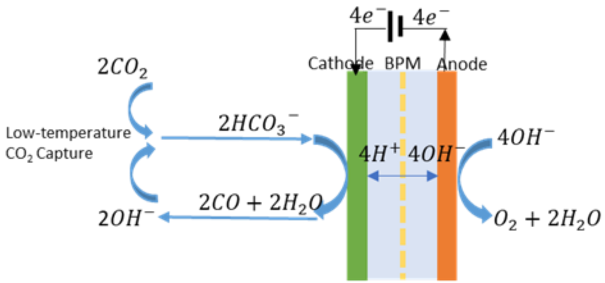
Reactive Capture Technology Categories



Electrochemical Pathway Overview

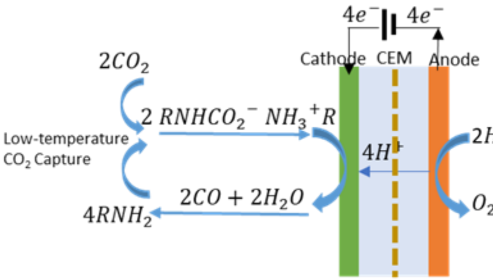
- *Primary Products*: CO, Syngas, Formate, and Solid Carbon (High-T)
- TRL: 2 – 3
- Current densities up to 200 mA/cm^2 have been demonstrated under some conditions
- Limited demonstration of DAC integration
- Small electrode surface areas (<10cm^2) and limited durability testing

Low-T (bi)carbonates



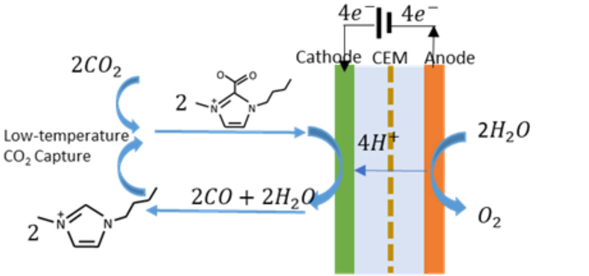
Ag/Hg/Pd, $KHCO_3$ / $NaHCO_3$, RT

Low-T Amines



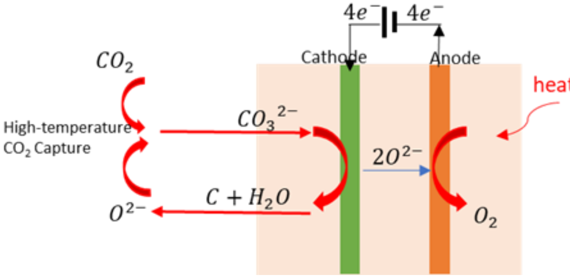
Ag/Cu/Bi/Pb, MEA/EDA, RT – 60°C

Low-T Ionic Liquids



Ag/Bi, [BMIM]/[EMIM], RT

High-T Molten Salts



Ni/Fe/Ti, Li_2CO_3, 500 - 900°C

Thermochemical Pathway Overview

- *Primary Products*: Methane, Syngas, Methanol, Formic Acid, and Carbonates
- TRL: 2 – 4
- Elevated temperature (and pressure)
- Opportunities for plasma-driven approaches
- DAC integration demonstrated for one-pot synthesis
- Often evaluated in batch mode with a limited number of cycles

Pathway		Reactants	Reaction	End-product
Dual Function Materials (DFM)		H_2, CO_2	320C, 1 bar MgO +(Ru + CeO_2)	Methane
Calcium looping		CH_4, CO_2	800C, 600C CaO + Ni	Syngas
One-pot system	Amine based	H_2, CO_2	170C, 60 bar Tertiary amine + EtOH + $Cu/ZnO/Al_2O_3$	MeOH
One-pot system	Cyclical carbonates	Ethylene oxide, CO_2	20C, 1.2 bar $NbCl_5$+NBu_4Br	Ethylene Carbonate
One-pot system	Cyclical carbonates	Propylene oxide, CO_2	50C, 5 bar $NbCl_5$+NBu_4Br	Propylene Carbonate
One-pot system	Amidine based	H_2, CO_2	25C, 60C, 160C, 4MPa+4MPa Amidine + $RhCl_3.3H_2O$ + MeOH + Biphosphene	Formic Acid
One-pot system	Hydroxide based	H_2, CO_2 (DAC)	140C, 70 bar KOH+ ethylene glycol l+ Ru-PNP	MeOH

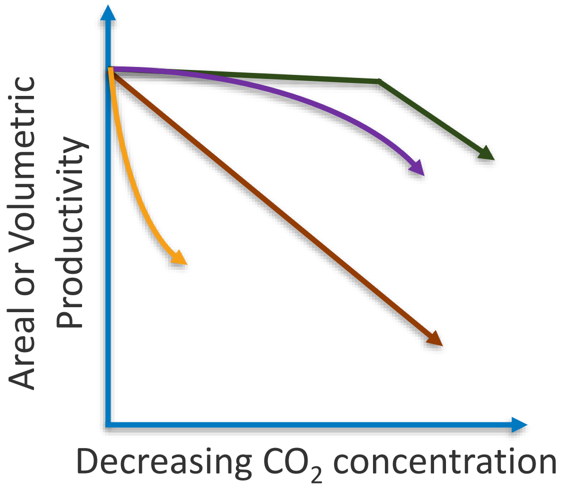
Biological Pathway Overview

- *Primary Products*: Methane, Ethanol, Acetate, Microalgae
- TRL: 2 – 9 (off-gases, power-to-gas)
- Diverse product slate accessible through metabolic engineering
- Mild temperature and pressure
- Methanogens and Acetogens are anaerobic microbes, thus DAC integration is challenging
- Mass transport limits productivity when considering low CO_2 concentrations

	Product	CO_2 conversion (%)	Selectivity (%)	Productivity (g/L/day)	T (℃); P(atm)	CO_2 Source
Microalgae	Chlorella sp.	60%	100%	0.682	26; 1	Air CO_2
	Chlorella valgaris	71%	100%	0.040	25; 1	Air CO_2
	Chlorella valgaris	45%	100%	0.024	25; 1	Air CO_2
	Scenedesmus obliquus	n.a.	100%	0.009	30; 1	Air CO_2
	Scenedesmus obliquus	n.a.	100%	0.016	30; 1	Air CO_2
	Scenedesmus sp	24%	100%	0.203	30; 1	Flue gas
	B. braunii	n.a.	100%	0.077	30; 1	Flue gas
Methanogen	Methane	99%	100%	568.9	62.5; 8.4	Biogas
	Methane	85%	100%	97.5	65; 4.9	Pure CO_2
	Methane	60%	100%	364.8	65; 4.9	Pure CO_2
	Methane	22%	100%	87.9	65; 0.74	Pure CO_2
	Methane	65%	100%	53.5	65; 0.74	Pure CO_2
Acetogen	Ethanol	95%	95%	195	37; 1	MSW gas
	2,3-BDO	95%	5%	14	37; 1	MSW gas
	Acetate	~100%	90%	148	30; 1	Pure CO_2

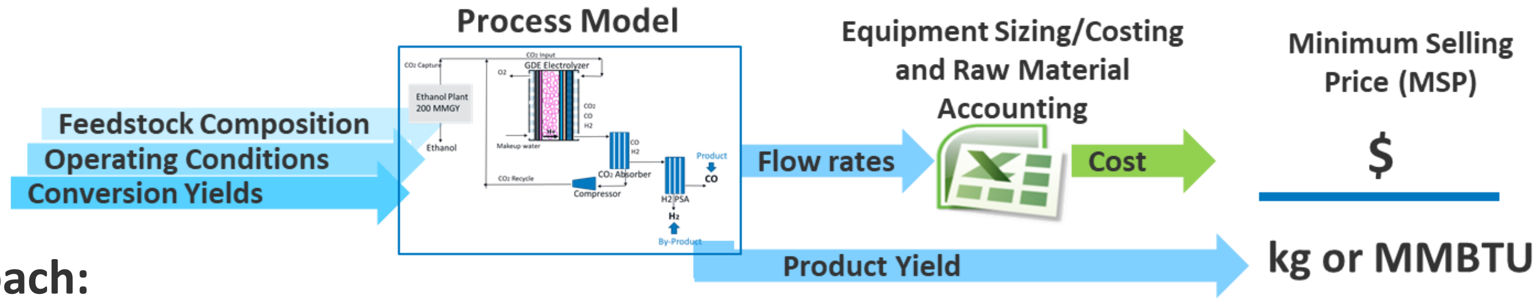
Overarching Challenges and Needs

- Integrating with real process streams
- Transitioning from batch to continuous processing – matching capture and conversion rates
- Understanding and mitigating impacts of impurities
- Quantifying capture media stability, attrition, and cycleability
- Identifying figures of merit
  - Energy efficiency
  - Productivity-normalized capex



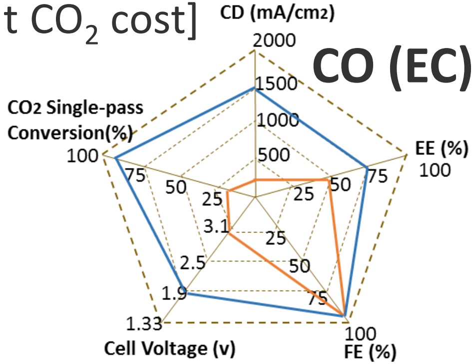
CO_2-to-Intermediates

Technoeconomic Analysis (TEA) Methodology



Approach:

- Design conceptual process including all major steps
- Calculate ***minimum selling price (MSP)*** using discounted cash-flow analysis (2016$)
- Evaluate 3 scenarios with major assumptions and technical metrics based on:
  - ***Current***: Results published in the open literature [$0.068/kWh; $40/mt CO_2 cost]
  - ***Future***: Attainable process improvements or engineering judgements [$0.03/kWh; $20/mt CO_2 cost]
  - ***Theoretical***: Thermodynamic limitations [$0.02/kWh; $0/mt CO_2 cost]
- Perform inclusive sensitivity analysis to identify:
  - Key cost drivers
  - R&D needs to realize cost reductions
- ***Scale basis:*** CO_2 stream generated from a 200M gallon per year ethanol biorefinery



Uncertainty and Interpretation

All analysis has associated uncertainty due to approach and input data

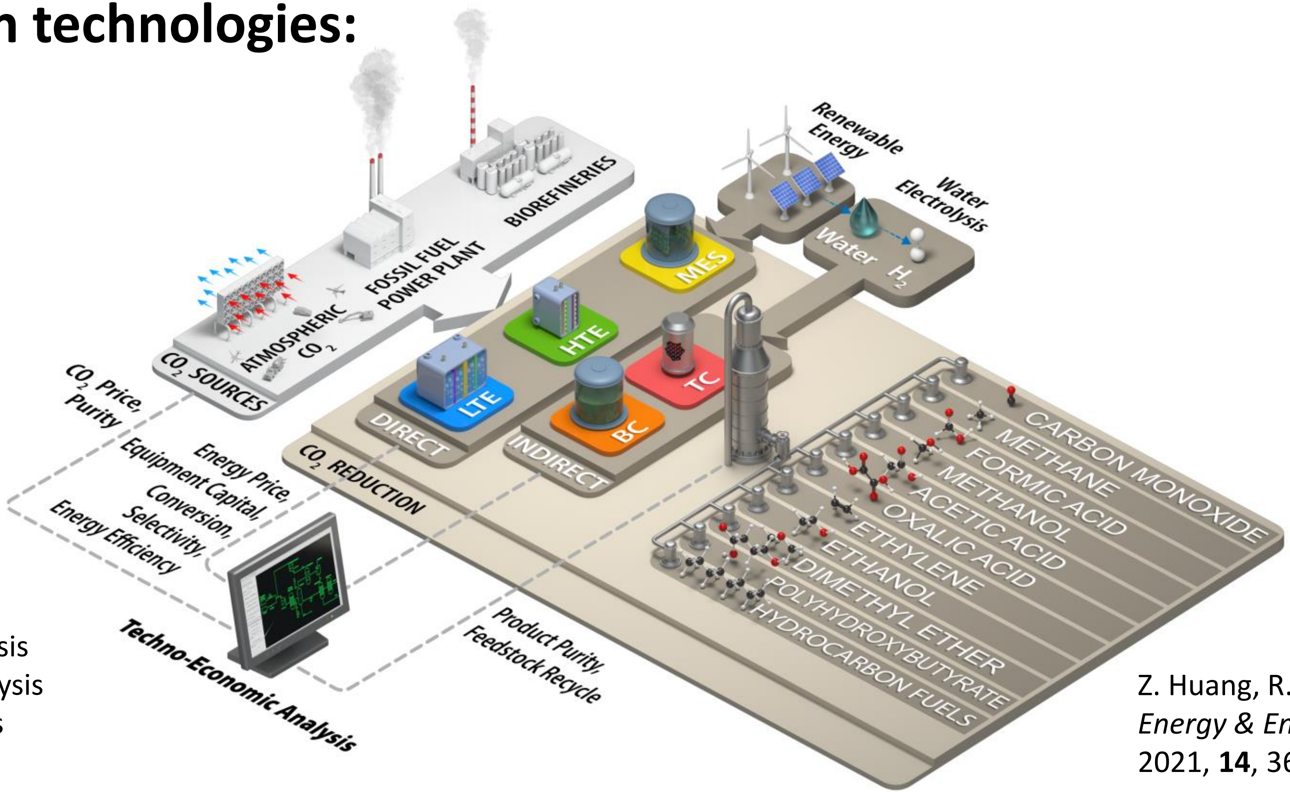
Definition	Purpose	Common Methodology	Expected Accuracy	Typical time requirement
Class 5	Concept screening	Scaled or by	High: +30 to +100%	Hours
Class 4				week up to a ew months
Class 3	Budget authorization	More detailed costs	Low: -10% to -20%	p to a year
Class 2	Bid estimates	Detailed unit designs and costs	High: +5 to +20% Low: -5% to -15%	More than a year
Class 1	Baseline cost of design	Based on actual design details of each unit	High: +3 to +15% Low: -3% to -10%	Several years worth of time

MSPs are cost estimates. They are not direct indicators or metrics for market relevance or commercial readiness.

AACE International Recommended Practice No. 18R-97

Selected Pathways and Products

Calculated MSP values for products across 5 different (direct and indirect) CO_2 reduction technologies:



LTE: Low-temperature electrolysis
HTE: High-temperature electrolysis
MES: Microbial Electrosynthesis
BC: Biochemical
TC: Thermochemical

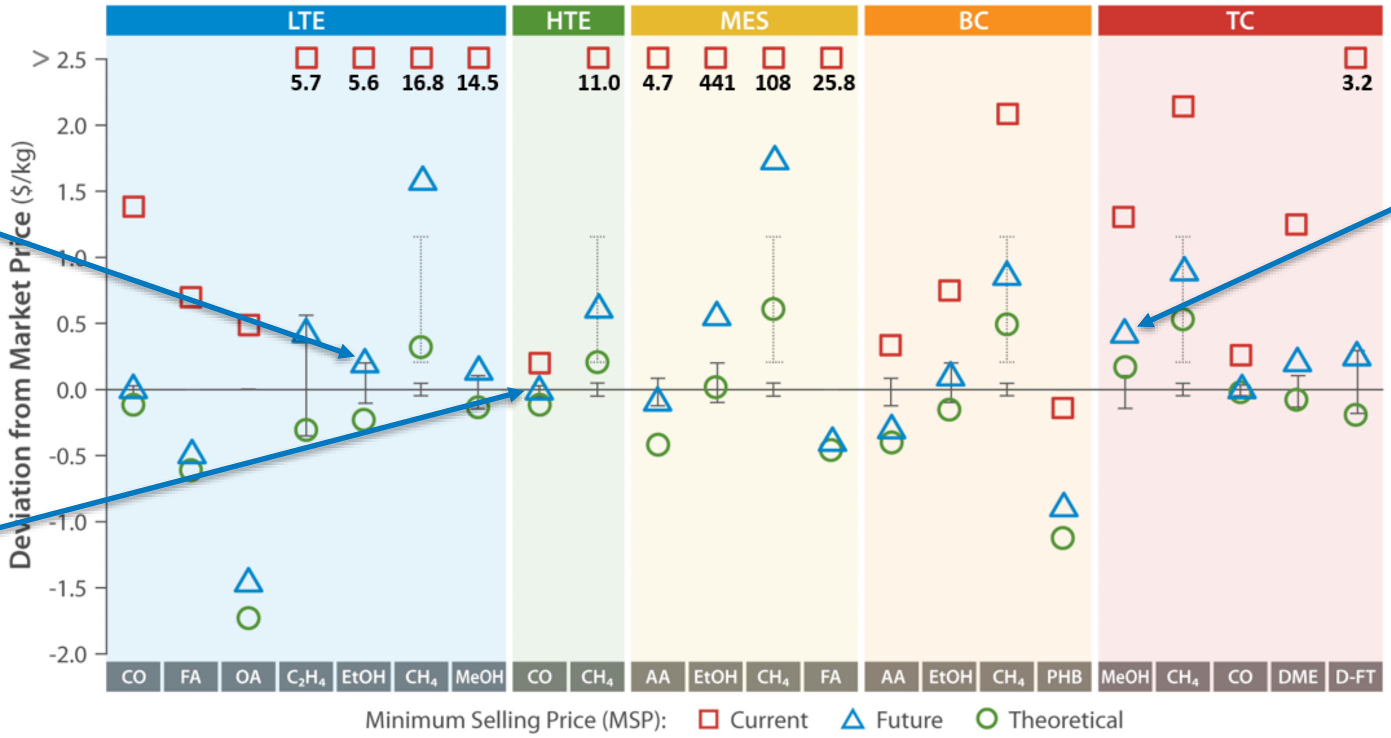
Z. Huang, R. Grim, et al., *Energy & Environ. Sci.*, 2021, **14**, 3664-3678.

Viability of Near-term Products

Economics are challenging under current conditions, but 8 of 11 products can reach market parity in future scenario

Ethanol
$0.74/kg
$27/GJ

CO
$0.15/kg
$15/GJ

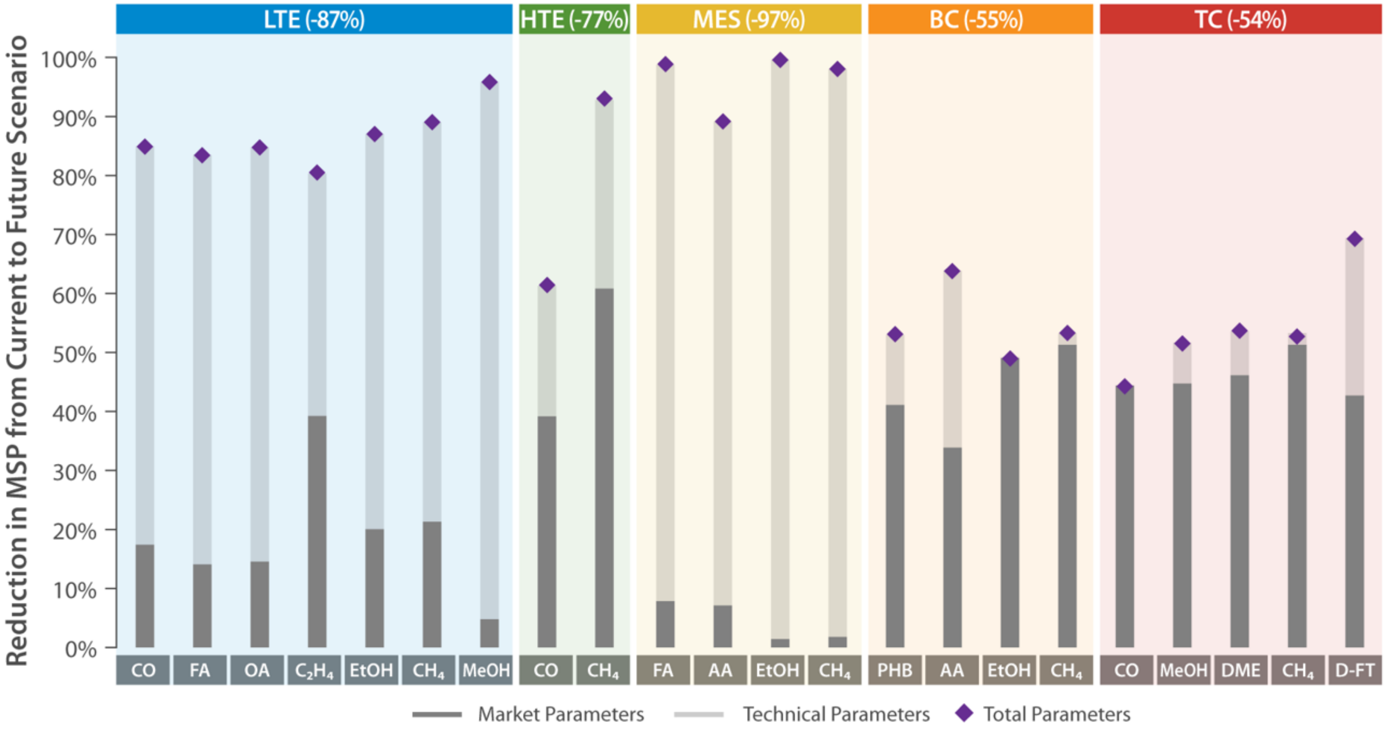


Methanol
$0.8/kg
$40/GJ

Z. Huang, R. Grim, et al., *Energy & Environ. Sci.*, 2021, **14**, 3664-3678.

Technology and Market Impacts

Opportunities exist for significant cost reduction through both favorable market conditions and technological advancements



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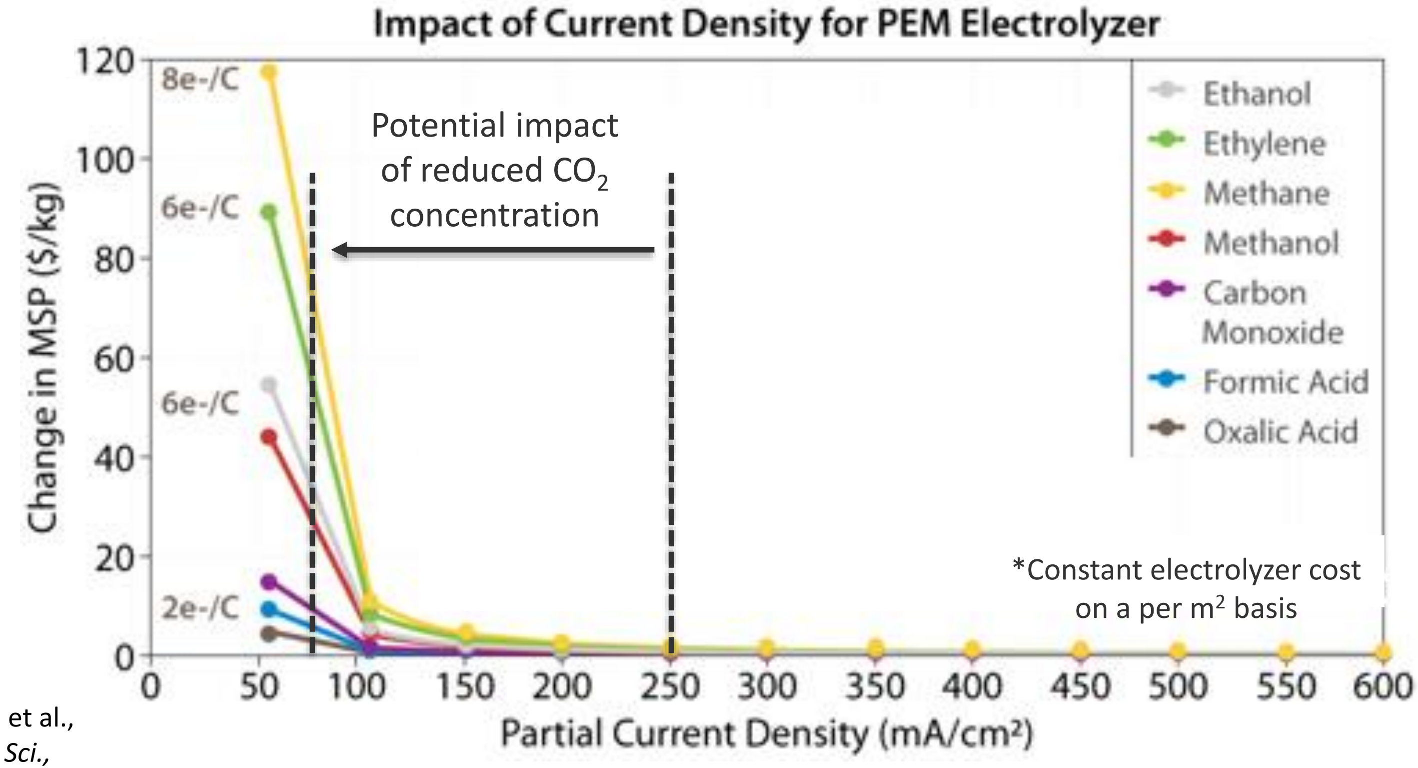
Opportunities for Transformational R&D

Economic analysis can help identify specific areas for transformational R&D



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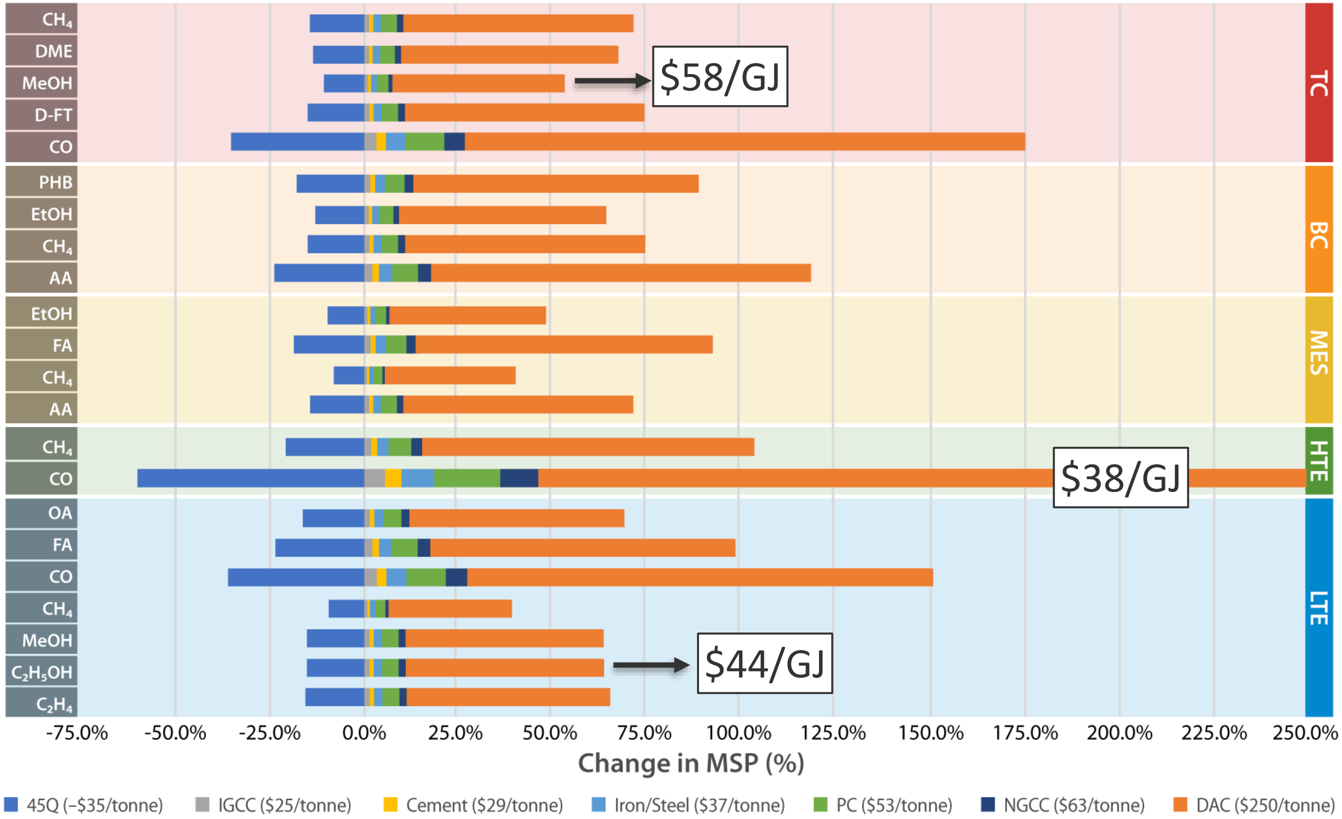
Impact of CO_2 Cost

CO_2 source plays a critical role in overall economic viability

- Energy efficient processes utilizing the fewest electrons exhibit the highest relative impact of CO_2 cost on MSP

- Increasing the CO_2 price from $20/tonne (baseline) to $63/tonne (NGCC) increases MSP on average about 15%



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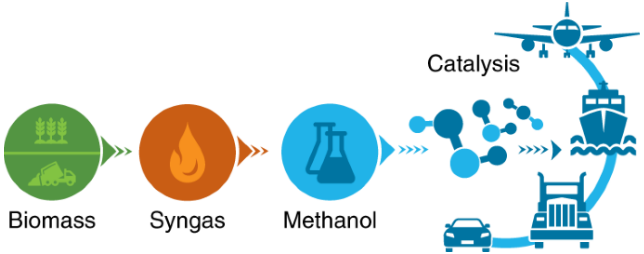
Interactive Visualization Website

https://www.nrel.gov/bioenergy/co2-utilization-economics/

Cost of Intermediate Upgrading

Methanol to High-Octane Gasoline



Estimated Cost:
$0.4 - $0.6/GGE
$3 - $5/GJ

D. Ruddy, et al., *Nature Catalysis,* 2019, **2**, 632-640.

Ethanol to SAF

Estimated Cost:
$0.9 - $1.2/GGE
$7 - $9/GJ

L. Tao, et al., *Green Chemistry,* 2017, **19**, 1082-1101.

Summary

- Reactive capture is still relatively early stage, but a multitude of technology options exist
  - Integration is essential combined with durability testing to prove out performance metrics
  - Rigorous TEA, LCA, systems analysis, and risk assessment can help guide development
- DAC-to-SAF can achieve significant carbon intensity reductions relative to petroleum jet fuel when leveraging low-C electricity
- Beyond electricity price, capex utilization and overall energy efficiency play a critical role in economic viability
- **How do we design technologies to drive down energy intensity while maximizing productivity?**

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Technology Manager: Ian Rowe

arpa·e CHANGING WHAT'S POSSIBLE

David Babson and Ian Robinson

Team members and contributors:

Ling Tao
Zhe Huang
Gary Grim
Dwarak Ravikumar
Mike Resch
Mike Guarnieri
Zhenglong Li (ORNL)
Dong Ding (INL)
Lesley Snowden-Swan (PNNL)
Jack Ferrell
Randy Cortright
Abhijit Dutta
Eric Tan
KC Neyerlin
Steve Phillips (PNNL)
Chirag Mevawala (PNNL)
Richard Boardman (INL)

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Thank You

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Joshua.Schaidle@nrel.gov

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